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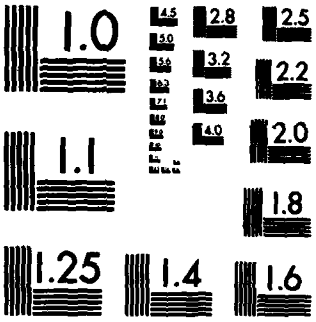
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Glassy Polymers, Nonlinear Problems, Continuum Mechanics, Bifurcation, Fluid Dynamics, Reaction-Diffusion Systems,

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The theory and application of bifurcation has been advanced in a wide array of problems in fluid dynamics and in reaction-diffusion systems. New models for diffusion in glassy polymers have been proposed and analyzed. New methods, both numerical and analytical, have been developed and applied to solving and analyzing bifurcation and other nonlinear problems. — and keywords include: —

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NONLINEAR PROBLEMS IN CONTINUUM MECHANICS

FINAL REPORT COVERING

1 August 1981 - 31 July 1984

D.S. Cohen and H.B. Keller

October 15, 1984

U. S. ARMY RESEARCH OFFICE

CONTRACT, DAAG29-81-K-0107

CALIFORNIA INSTITUTE OF TECHNOLOGY

Brief Summary of Research Program

The program on nonlinear problems in continuum mechanics during the past three years has been extremely productive. We have advanced the theory and application of bifurcation in a wide array of problems in fluid dynamics and in reaction-diffusion systems. New models for diffusion in glassy polymers have been proposed and analyzed. We have developed and applied new methods, both numerical and analytical, for solving and analyzing bifurcation and other nonlinear problems. We have trained a variety of students and post-docs in broad areas of applied mathematics, most specifically in nonlinear problems related to the goals of this program. At least five Ph.D. students have been produced during this period working primarily on problems of direct interest to this program. Visitors and post-docs from overseas have also been involved throughout the work and tenure of this program.

A brief outline of the results obtained under this program is contained in the following brief summaries of our publications, preprints and Ph.D. theses. A bibliography of published, submitted and papers in preparation is included in the outline. We also list the scientific personnel supported under this program and the Ph.D. degrees awarded during the current contract period.

Publications and Summaries of Work

1. Two New Bifurcation Phenomena, H.B. Keller in Applications of Nonlinear Analysis in the Physical Sciences (eds. H. Amonn, K. Kirchgassner, N. Basley) Pitman Pubs., London 1981 (60-73).

   We examine here two new bifurcation phenomena, namely isola formation and multiple limit point bifurcation. The former phenomenon has been observed many times in specific problems and indeed is even discussed in the literature. But we show here its intimate connection with perturbed bifurcation theory. The obvious analogy with hyperbolic -- and elliptic -- points is clearly apparent. The work on isola formation is the result of discussions with B. Matkowski and E. Reiss who have a somewhat different approach using singular perturbations.

2. Path Following Near Bifurcation, D.W. Decker and H.B. Keller, C.P.A.M. 34, 1981 (149-175).

   Constructive methods for computing and/or analyzing solution paths of problems in the form

   $$G(u,\lambda) = 0 , \quad G, u \in \mathbb{B}, \quad \lambda \in \mathbb{R}$$

   are studied. In particular the behavior near folds and bifurcation points is examined. It is shown that the inflation technique we have previously introduced improves the domain of convergence even though it may not always eliminate the singularity. Surprisingly higher dimensional null spaces seem to yield more robust convergence cones (i.e. broader angles at the cusp) than the one-dimensional case.

3. Geometrically Isolated Nonisolated Solutions and their Approximation, H.B. Keller, SIAM J. Numer. Anal., v.18, n.5, 1981 (822-838).

   A solution $x = x^0$ of $F(x) = 0$ is said to be "isolated" if the Frechet derivative $F'(x^0)$ is nonsingular. It is said to be "geometrically isolated" if no other solution is in $\|x - x^0\| \leq \rho$ for some $\rho > 0$. Isolated solutions are always geometrically isolated. Sufficient conditions are obtained to insure that a nonisolated solution is also geometrically isolated. We then study the application of approximation methods, in the general form $F_h(x_h) = 0$, to approximate nonisolated solutions which are geometrically isolated. Under strong consistency conditions the results are somewhat negative -- the approximations may have an even number (including zero) or an odd number of roots near x^0, depending upon the "multiplicity" of x^0 as a root. If the accuracy is $O(h^p)$ and the multiplicity is N, then the approximations have error $O(h^{p/N})$. The relation of these results to limit and bifurcation points is discussed briefly.

4. Continuation Methods in Computational Fluid Dynamics, in Numerical & Physical Aspects of Aerodynamic Flows (ed. T. Cebeci), Springer-Verlag, New York, 1982 (3-13).

Continuation methods are extremely powerful techniques that aid in the numerical solution of nonlinear problems. Their use in computational fluid dynamics has, until very recently, been minimal. This is somewhat surprising, since they are rather well known in solid mechanics. Furthermore, their mathematical foundations -- homotopy methods -- were laid by mathematicians very much concerned with fluid-dynamical problems and in particular with the construction of existence proofs for the Navier-Stokes equations. We shall attempt here to recall or expose some of these ideas and to indicate some of their current uses in computational fluid dynamics.

5. Invariant Imbedding, the Box Scheme and an Equivalence between Them, H.B. Keller and M. Lentini, SIAM J. Numer. Anal., v.19, n.5, 1982 (942-962).

We show (for general linear two-point boundary value problems) that the box scheme and invariant imbedding are equivalent in the sense that a specific algorithm for solving the difference equations is valid if and only if an appropriate imbedding is valid. A key element in the equivalence is the role played by pivoting to solve the linear equations and "switching" to get a finite imbedding. Part of the equivalence proof shows that imbedding is the completion of the box scheme. Multiple imbeddings are introduced and a lower bound for the critical length problem is obtained.

6. On the Birth of Isolas, D. Dellwo, H.B. Keller, B.J. Matkowsky and E.L. Reiss, SIAM J. Appl. Math., v.42, n.5, 1982 (956-963).

Isolas are isolated, closed curves of solution branches of nonlinear problems. They have been observed to occur in the buckling of elastic shells, the equilibrium states of chemical reactors and other problems. In this paper we present a theory to describe analytically the structure of a class of isolas. Specifically, we consider isolas that shrink to a point as a parameter τ of the problem, approaches a critical value τ_0. The point is referred to as an isola center. Equations that characterize the isola centers are given. Then solutions are constructed in a neighborhood of the isola centers by perturbation expansions in a small parameter ε that is proportional to $(\tau-\tau_0)^\alpha$, with α appropriately determined. The theory is applied to a chemical reactor problem.

7. Arc-Length Continuation and Multi-Grid Techniques for Nonlinear Elliptic Eigenvalue Problems, T.F.C. Chan and H.B. Keller, SIAM J. Sci. Stat. Comput. v.3, n.2, 1982 (173-194).

We investigate multi-grid methods for solving linear systems arising from arc-length continuation techniques applied to nonlinear elliptic eigenvalue problems. We find that the usual multi-grid methods diverge in the neighborhood of singular points of the solution branches. As a result, the continuation method is unable to continue past a limit point in the Bratu problem. This divergence is analyzed and a modified multi-grid algorithm has been devised based on this analysis. In principle, this new multi-grid algorithm converges for elliptic systems arbitrarily close to singularity and has been used successfully in conjunction with arc-length continuation procedures on the model problem. In the worst situation, both the storage and the computational work are only about a factor of two more than the unmodified multi-grid methods.

8. Practical Procedures in Path Following Near Limit Points, in Computing Methods in Applied Sciences and Engineering VI (eds. R. Glowinski & J.L. Lions) North-Holland, New York 1982 (177-183).

The computation of solution paths of general nonlinear problems in the form

$$G(u,\lambda) = 0 , \quad G, u \in \mathbb{R}^N, \quad \lambda \in \mathbb{R}$$

near folds or limit points is studied. In particular singular and near singular linear systems must be solved. We study the Bordering Algorithm -- a special form for block Gaussian elimination -- for doing this. With appropriate pivoting it is shown that the method works even in the singular case. Some loss in accuracy due to cancellation of significant digits is to be expected. The analysis also shows efficient ways to compute both left and right null vectors of a singular matrix.

9. Driven Cavity Flows by Efficient Numerical Techniques, R. Schreiber and H.B. Keller, J.C.P., v.49, n.2, 1983 (310-333).

Efficient and reliable numerical techniques of high-order accuracy are presented for solving problems of steady viscous incompressible flow in the plane, and are used to obtain accurate solutions for the driven cavity. A solution is obtained at Reynolds number 10,000 on a 180 x 180 grid. The numerical methods combine an efficient linear system solver, an adaptive Newton-like method for nonlinear systems, and a continuation procedure for following a branch of solutions over a range of Reynolds numbers.

10. Spurious Solutions in Driven Cavity Calculations, R. Schreiber and H.B. Keller, J.C.P., v.29, n.1, 1983 (165-172).

    Spurious numerical solutions of the Navier-Stokes equations occur frequently. It is not always clear how to identify the "proper" and "spurious" solutions. Some aspects of these difficultles are discussed. Indeed it seems clear that more spurious solutions are to be expected than proper ones. Examples from the famous driven cavity flow are given and numerous spurious solutions reported as proper in the literature are exposed.

11. Convergence Rates for Newton's Method at Singular Points, D.W. Decker, H.B. Keller and C.T. Kelley, SIAM J. Numer. Anal. v.20, n.2, 1983 (296-314).

    If Newton's method is employed to find a root of a map from a Banach space into itself and the derivative is singular at that root, the convergence of the Newton iterates to the root is linear rather than quadratic. In this paper we give a detailed analysis of the linear convergence rates for several types of singular problems. For some of these problems we describe modifications of Newton's method which will restore quadratic convergence.

12. The Bordering Algorithm and Path Following Near Singular Points of Higher Nullity, H.B. Keller, SIAM J. Sci. Stat. Comput., v.4, n.4, 1983 (573-582).

    We study the behavior of the bordering algorithm (a form of block elimination) for solving nonsingular linear systems with coefficient matrices in the partitioned form $\begin{pmatrix} A & B \\ C^* & D \end{pmatrix}$ when $\dim \mathcal{N}(A) \geq 1$. Systems with this structure naturally occur in path following procedures. We show that under appropriate assumptions, the algorithm, which is based on solving systems with coefficient matrix A, works as A varies along a path and goes through singular points. The required assumptions are justified for a large class of problems coming from discretizations of boundary value problems for differential equations.

13. The Stability of One-Step Schemes for First-Order Two-Point Boundary Value Problems, C. de Boor, F. de Hoog and H.B. de Keller, SIAM J. Numer. Anal., v.20, n.6, 1983 (1139-1146).

The stability of a finite difference scheme is related explicitly to the stability of the continuous problem being solved. At times, this gives materially better estimates for the stability constant than those obtained by the standard process of appealing to the stability of the numerical scheme for the associated initial value problem.

14. Fast Seismic Ray Tracing, H.B. Keller and D.J. Perozzi, SIAM J. Appl. Math., v.43, n.4 1983 (981-992).

New methods for the fast, accurate and efficient calculation of large classes of seismic rays joining two points x_S and x_R in very general two-dimensional configurations are presented. The medium is piecewise homogeneous with arbitrary interfaces separating regions of different elastic properties (i.e., differing wave speeds c_p and c_S). In general there are 2^{N+1} rays joining x_S to x_R while making contact with N interfaces. Our methods find essentially all such rays for a given N by using continuation or homotopy methods on the wave speeds to solve the ray equations determined by Snell's law. In addition travel times, ray amplitudes and caustic locations are obtained. When several receiver positions $x_R^{(j)}$ are to be included, as in a gather, our techniques easily yield all the rays for the entire gather by employing continuation in the receiver location. The applications, mainly to geophysical inverse problems, are reported elsewhere.

15. Steady State and Periodic Solution Paths: their Bifurcations and Computations, H.B. Keller and A.D. Jepson, to appear in: Numerical Methods for Bifurcation Problems (eds. T. Kupper, H.D. Mittleman) ISNM Series, Berkhauser Verlag, Basel, 1984.

A brief account of the theory and numerical methods for the analysis and solution of nonlinear autonomous differential equation systems is given. Path methods for generating steady states are first summarized. Then it is shown how to reduce the periodic case to that of steady state type calculations. Hopf bifurcations and folds in periodic solution paths are treated. Direct methods for finding Hopf bifurcation points are given. Some results from "fold following" are presented.

16. Numerical Methods for Hopf Bifurcation and Continuation of Periodic Solutions Paths, E.J. Doedel, A.D. Jepson and H.B. Keller, in: Computing Methods in Applied Sciences and Engineering VI (eds. R. Glowinski, J.-L. Lions), North Holland, Amsterdam, 1984 (127-138).

Path following techniques for steady state problems are readily extended to apply to periodic solutions of autonomous systems. Fold points and bifurcations are easily determined. In addition paths of singular points -- folds, simple bifurcations, Hopf bifurcations -- that occur in multiparameter problems are computed directly. This is basically a survey of known methods devised and applied by the authors.

17. Continuation-Conjugate Gradient Methods for the Least Squares Solution of Nonlinear Boundary Value Problems, R. Glowinski, H.B. Keller and L. Reinhart, SIAM J. Sci. & Stat. Comp., 1984, in press.

We discuss in this paper a new combination of methods for solving nonlinear boundary value problems containing a parameter. Methods of the continuation type are combined with least squares formulations, preconditioned conjugate gradient algorithms and finite element approximations.

We can compute branches of solutions with limit points, bifurcation points, etc.

Several numerical tests illustrate the possibilities of the methods discussed in the present paper; these include the Bratu problem in one and two dimensions, one-dimensional bifurcation and perturbed bifurcation problems, the driven cavity problem for the Navier-Stokes equations.

18. Some Bifurcation Diagrams for Taylor Vortex Flows, Rita Meyer-Spasche and H.B. Keller, submitted to Phys. of Fluids, 1984.

The numerical continuation and bifurcation methods of Keller [H.B. Keller, in Applications of Bifurcation Theory, (Academic Press, New York 1977) pp. 359-384] are used to study the variation of some branches of axisymmetric Taylor vortex flow as the wavelength in the axial direction changes. Closed "loops" of solutions and secondary bifurcations are determined. Variations with respect to Reynolds number show the same phenomena.

Our results show that Taylor vortices with periodic boundary conditions exist in a wider range of wavelengths, λ, than observed in the Burkhalter/

Koschmieder experiments [Phys. Fluids 17, 1929 (1974)]. They also show that there is possibly a λ-subinterval within the neutral curve of Couette flow such that there are no Taylor vortex flows with smallest period in this interval.

19. A Multigrid Continuation Method for Elliptic Problems with Turning Points, J.H. Bolstad and H.B. Keller, submitted to SIAM J. Sci. & Stat. Comp., 1984.

We introduce a new multigrid continuation method for computing solutions of nonlinear elliptic eigenvalue problems which contain limit points (also called turning points or folds). Our method combines the frozen tau technique of Brandt with pseudo-arc length continuation and correction of the parameter on the coarsest grid. This produces considerable storage savings over direct continuation methods, as well as better initial coarse grid approximations, and avoids complicated algorithms for determining the parameter on finer grids. We provide numerical results for second, fourth and sixth order approximations to the two-parameter, two-dimensional stationary reaction-diffusion problem:

$$\Delta u + \lambda \exp(u/(1+au)) = 0 .$$

For the higher order interpolations we use bicubic and biquintic splines. The convergence rate is observed to be independent of the occurrence of limit points.

20. A Generalized Diffusion Model for Growth and Dispersal in a Population, D.S. Cohen and J.D. Murray, J. Math Biology, 12, 1981 (237-249).

A reaction-diffusion model is presented in which spatial structure is maintained by means of a diffusive mechanism more general than classical Fickian diffusion. This generalized diffusion takes into account the diffusive gradient (or gradient energy) necessary to maintain a pattern even in a single diffusing species. The approach is based on a Landau-Ginzburg free energy model. A problem involving simple logistic kinetics is fully analyzed, and a nonlinear stability analysis based on a multi-scale perturbation method shows bifurcation to non-uniform states.

21. A Delay Logistic Equation with Variable Growth Rate, D.S. Cohen and S. Rosenblat, SIAM J. Appl. Math, v.42, n.3, 1982 (608-624).

A logistic equation with distributed delay is considered in the case where the growth rate oscillates sinusoidally about a positive mean value. A delay kernel is chosen which admits bifurcation of the equilibrium state into a periodic solution when the growth rate is constant. It is shown that the fluctuations in growth rate modulate the bifurcation into a quasiperiodic solution. In certain circumstances, however, it is shown that frequency locking can occur but that this is a local phenomenon which does not persist outside the immediate vicinity of the bifurcation point.

22. Waiting-Time Behavior in a Nonlinear Diffusion Equation, W.L. Kath and D.S. Cohen, Stud. in Appl. Math, 67, 1982 (79-105).

We study the nonlinear diffusion equation $u_{t^*} = (u^n u_x)_x$, which occurs in the study of a number of problems. Using singular-perturbation techniques, we construct approximate solutions of this equation in the limit of small n. These approximate solutions reveal simply the consequences of this variable diffusion coefficient, such as the finite propagation speed of interfaces and waiting-time behavior (when interfaces wait a finite time before beginning to move), and allow us to extend previous results for this equation.

23. Gaseous Diffusion in Glassy Polymers, D.S. Cohen and E.A. Stanley, SIAM J. Appl. Math., v.43, n.4, 1983 (949-970).

A model for gaseous diffusion in glassy polymers is developed with a view to accounting for the observations made in dual sorption and certain other phenomena in polymers below their glass transition temperature. In this paper a preliminary study of the effects of both the immobilizing mechanism and the generalized diffusion mechanism on travelling waves and the diffusive wavefronts is made.

24. Imperfect Bifurcation Near a Double Eigenvalue: Transitions between Nonsymmetric and Symmetric Patterns, T. Erneux and D.S. Cohen, SIAM J. Appl. Math., v.43, n.5, 1983 (1042-1060).

We examine the existence of nonsymmetric and symmetric steady state solutions of a general class of reaction-diffusion equations.

Our study consists of two parts:

(i) By analyzing the bifurcation from a uniform reference state to nonuniform regimes, we demonstrate the existence of a unique symmetric solution (basic wave number two) which becomes linearly stable when it surpasses a critical amplitude. (We assume that the first bifurcation point corresponds to the emergence of the simplest nonsymmetric steady state solutions.)

(ii) This result is not affected when a parameter is nonuniformly distributed in the system. However, one of the two possible branches of nonsymmetric solutions may disappear from the bifurcation diagram.

Our analysis is motivated by the fact that experimental observations of pattern transitions during morphogenesis are interpreted in terms of the dynamics of stable concentration gradients. We have shown that in addition to the values of the physico-chemical parameters, these structures can be selected by two different mechanisms:

(i) the linear stability of the nonuniform patterns,

(ii) the effects of a small and nonuniform variation of a parameter in the spatial domain..

25. Transitions between Nonsymmetric and Symmetric Steady States near a Triple Eigenvalue, D.S. Cohen and T. Erneux, SIAM J. Appl. Math., v.43, n.5, 1983 (1061-1074).

We examine the existence of nonuniform steady-state solutions of a certain class of reaction-diffusion equations. Our analysis concentrates on the case where the first bifurcation is near a triple eigenvalue. We derive the conditions for a continuous transition between nonsymmetric and symmetric solutions when the bifurcation parameter progressively increases from zero. Finally, we give an example of a four variables model which presents the possibility of a triple eigenvalue.

26. Theoretical Models for Diffusion in Glassy Polymers, D.S. Cohen, J. Polymer Sci., 21, 1983 (2057-2065).

A model is derived which incorporates and unifies many of the diverse observations occuring in diffusion in glassy polymers. This unification is made possible by explicitly formulating the common property of a glassy polymer in all its various modes, namely the finite relaxation time due to its slow response to changing conditions. The application and use of the model in various situations is discussed.

27. Theoretical Models for Diffusion in Glassy Polymers. II. D.S. Cohen, J. Polymer Sci., 22, 1984 (1001-1009).

The author refines and generalizes a model for diffusion in glassy polymers which he previously introduced. The model unifies many diverse observations by explicitly formulating the common property of a glassy polymer in all its various modes, namely the finite relaxation time due to its slow response to changing conditions. An integral approximation method is used to study the motion of the penetrant front and the glass-gel interface and a useful polynomial approximation method is introduced for use in special simple situations.

Ph.D. Degrees Awarded in Related Research

The following people worked on this program while graduate students and obtained their Ph.D. degrees in Applied Mathematics at Caltech. Their thesis titles are listed.

1. W.L. Kath, Ph.D. in Applied Mathematics, Caltech, 1981,
   I: Propagating and Waiting Fronts in Nonlinear Diffusion
   II: Sustained Reentry Roll Resonance

2. A.D. Jepson, Ph.D. in Applied Mathematics, Caltech, 1981,
   I: Asymptotic Boundary Conditions for Ordinary Differential Equations
   II: Numerical Hopf Bifurcation

3. J.R. Mueller, Ph.D. in Applied Mathematics, Caltech, 1982,
   I: The Analysis of the Rewetting of a Vertical Slab Using a Weiner-Hopf Technique
   II: Asymptotic Expansions of Integrals with Three Coalescing Saddle Points

4. J.A. Fawcett, Ph.D. in Applied Mathematics, Caltech, 1983,
   I: Three dimensional ray-tracing and ray inversion in layered media
   II: Inverse scattering and curved ray tomography with applications to seismology

5. T.M. Hagstrom, Ph.D. in Applied Mathematics, Caltech, 1983,
   Reduction of unbounded domains to bounded domains for partial differential equation problems

Other Personnel Supported by this Program

Research Associates

Dr. J.H. Bolstad
Dr. D.Brown
Dr. K.A. Cliff
Prof. E. Doedel
Dr. J. Goodrich
Dr. R. Meyer-Spasche
Dr. G. Schrauf
Dr. Z. Yang

Student Research Assistants

M. Brewster	C. Goodhart	J. Mueller
T. Colvin	T. Hagstrom	D. Rollins
J. Fawcett	M. Henderson	D. Schwendeman
J. Fier	A. Jepson	E.A. Stanley
T. Girnius	W. Kath	

Visitors

Dr. E. Ben-Jacob (I.T.P., Santa Barbara)
Professor F. Brezzi (U. Pavia, Italy)
Professor F. de Hoog (C.S.I.R.O., Australia)
Professor E. Doedel (Concordia U., Montreal)
Dr. N. Goldenfeld (I.T.P., Santa Barbara)
Dr. P. Hagan (Exxon)
Professor P. Kloeden (Australia)
Professor B. Matkowsky (Northwestern)
Professor R. Mattheij (Netherlands)
Dr. R. Meyer-Spasche (MPI, Garching, Germany)
Professor J. Murray (Oxford)

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